Physical Chemistry

CHANNELING LITHIUM THROUGH A SOLID ELECTROLYTE: AN NMR STUDY

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Very few *in-situ* studies have been performed on lithium ion batteries. We have developed the Coin Cell Battery Imager device for recording NMR spectra of each electrode during the electrochemical charge and discharge process. The NMR spectra are used to identify the Li-7 NMR chemical signatures for all lithium species in the electrochemical cell, and to investigate the transport of lithium ions in novel electrolyte materials. Coin type cells were assembled to study the proposed solid-state electrolyte dilithium phthalocyanine (DiLiPc). Lithium metal was used as the positive electrode, and a copper disk (NMR detector) served as the negative electrode. Galvanostatic cycling was performed between 1.5 and 0.0 V with a constant charge and discharge current of 1.0 mA. The NMR spectra obtained reveal that lithium ions insert into, but do not transport through the DiLiPc. We suspect that the DiLiPc is initially saturated with lithium ions before it can transport the lithium through the cell. Our current experiments use excess lithium metal to saturate the DiLiPc to the point where lithium transport can occur. The spectra in Figure 1 show the Li-7 NMR chemical signatures for the cell.

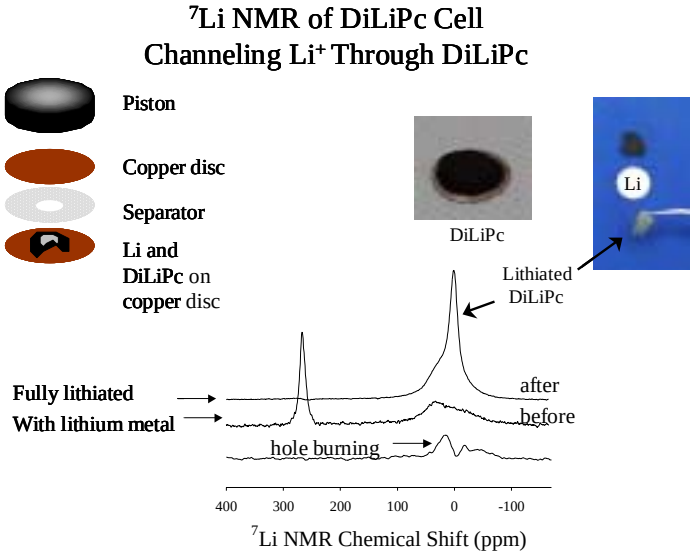

Figure 1. *In situ* Li-7 NMR spectra of the components of a lithium-ion electrochemical cell. The peak at 275 ppm is assigned to metallic lithium. The broad peak near 0 ppm indicates the presence of lithium in the solid electrolyte (DiLiPc) *before* the lithiation process. The Li-7 NMR spectrum recorded *after* the electrochemical insertion of lithium ions into DiLiPc reveals a new peak superimposed on the broad peak near 0 ppm. The bottom trace (obtained from a hole burning experiment) demonstrates that the peak is inhomogeneously broadened. The assembly of the cell components is shown on the left side of the figure. A photograph of the DiLiPc before and after lithiation is shown on the right side of the figure.